(FILE 'HOME' ENTERED AT 15:10:45 ON 11 MAY 2004)

FILE 'REGISTRY' ENTERED AT 15:11:01 ON 11 MAY 2004

L1 STRUCTURE UPLOADED

12 S L1 L2

214 S L1 SSS FULL Ľ3

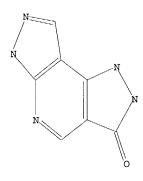
FILE 'CAPLUS' ENTERED AT 15:12:10 ON 11 MAY 2004

10 S L3 L4

=> d 11

L1 HAS NO ANSWERS

L1



Structure attributes must be viewed using STN Express query preparation.

#### => d 1-10 bib abs hitstr

ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN L4

2004:182530 CAPLUS AN

DN 140:235704

Preparation of dihydrodipyrazolopyridinones as B7-1/CD28 binding inhibitors for the immunotherapeutic treatment of organ transplant rejection

Green, Neal Jeffrey; Tam, Steve Yikkai; Xiang, Jason Shaoyun; Davies, Audrey Molina; Chen, Lihren; Stack, Gary Paul IN

Wyeth, John, and Brother Ltd., USA PΑ

U.S. Pat. Appl. Publ., 18 pp. so

CODEN: USXXCO

DTPatent

LA English

FAN.CNT 1					
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004044024	A1	20040304	US 2003-629227	20030728
PRAI	US 2002-399161P	P	20020729		

OS MARPAT 140:235704

Air off

Title compds. I [R1, R4 = H, (un) substituted alkyl, (un) substituted Ph, e.g., halo, OH, haloalkyl, etc.; R2 = H, (un) substituted alkyl, (un) substituted Ph, e.g., halo, NO2, CN, etc.; R3 = (un) substituted Ph, cycloheteroalkyl, heteroaryl, etc.], and their pharmaceutically acceptable salts were prepared For example, intramol. cyclization of compound II [ R1 = H; R2 = 3-FC6H4; R3 = 5-bromopyrid-3-yl; R4 = CH3], e.g., prepared from Et 5-amino-1-methyl-4-pyrazolecarboxylate in 3-steps, afforded compound I [ R1 = H; R2 = 3-FC6H4; R3 = 5-bromopyrid-3-yl; R4 = CH3] in 93% yield. In B7-1/CD28 binding inhibition assays, 75-examples of compds. I exhibited IC50 values ranging from 4-3000 nM, e.g., the IC50 value of compound I [R1 = H; R2 = 3-FC6H4; R3 = 5-bromopyrid-3-yl; R4 = CH3] was 20 nM. Of note, dihydrodipyrazolopyridinone I is useful for the immunotherapeutic treatment of transplant rejection and autoimmune diseases. 443146-92-7P 443146-93-8P 635324-71-9P 635324-72-0P 635324-73-1P 635324-75-3P 635324-76-4P 635324-79-7P 635324-82-2P 635324-84-4P 635324-85-5P 635324-87-7P 635324-90-2P 635324-92-4P 635324-93-5P 635324-94-6P 635324-95-7P 635324-96-8P 635324-97-9P 635324-98-0P 635324-99-1P 635325-03-0P 635325-05-2P 635325-06-3P 635325-07-4P 635325-09-6P 635325-11-0P 635325-19-8P 635325-20-1P 635325-21-2P 635325-23-4P 635325-25-6P 635325-27-8P 635325-28-9P 635325-29-0P 635325-30-3P 635325-31-4P 635325-32-5P 635325-34-7P 635325-35-8P 635325-36-9P 635325-37-0P 635325-38-1P 635325-77-8P 635325-95-0P 668481-76-3P 668481-77-4P 668481-78-5P 668481-79-6P 668481-80-9P 668481-81-0P 668481-82-1P 668481-83-2P 668481-84-3P

668482-04-0P 668482-06-2P 668482-07-3P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

668481-85-4P 668481-86-5P 668481-87-6P 668481-88-7P 668481-89-8P 668481-90-1P 668481-91-2P 668481-92-3P 668481-93-4P 668481-95-6P 668481-97-8P 668481-97-6P 668481-97-6P 668481-97-0P 668482-00-6P 668482-01-7P 668482-03-9P

RN

CN

(preparation of dihydrodipyrazolopyridinones as B7-1/CD28 binding inhibitors for the immunotherapeutic treatment of organ transplant rejection)
443146-92-7 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 443146-93-8 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME) CN

RN

635324-71-9 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-phenyl-CN4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

635324-72-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

635324-73-1 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN 635324-75-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-76-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]-2-[4-(trifluoromethyl)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$F_3$$
C N N Me

RN 635324-79-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(1,6-dihydro-6-oxo-3-pyridazinyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

635324-82-2 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[4-(1,1-dimethylethyl)phenyl]-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

RN

635324-84-4 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-[4-(phenylmethoxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

635324-85-5 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[1,1'-biphenyl]-4-yl-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

635324-87-7 CAPLUS RN

Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

$$HO_2C$$
 $H$ 
 $N$ 
 $N$ 
 $Me$ 

RN 635324-90-2 CAPLUS
CN Benzonitrile, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME)

RN 635324-92-4 CAPLUS
CN Benzoic acid, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME)

RN 635324-93-5 CAPLUS
CN Benzamide, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 635324-94-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635324-95-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 635324-96-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-aminophenyl)-2-(4-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635324-97-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-phenyl- (9CI) (CA INDEX NAME)

RN 635324-98-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-4-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

635324-99-1 CAPLUS RNDipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-pyridinyl)- (9CI) (CA INDEX NAME) CN

RN

635325-03-0 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3,5-dichlorophenyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN

635325-05-2 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-thienyl)- (9CI) (CA INDEX NAME) CN

635325-06-3 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-CN4-(3-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-07-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(1,3-benzodioxol-5-yl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-09-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridine-3,4-dione, 2-(3-fluorophenyl)-1,2,5,6-tetrahydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-11-0 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(2,6-dimethyl-4-morpholinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-19-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-phenyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-20-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-21-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,5-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-23-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-2-(4-fluorophenyl)-1,6-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-25-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro6-propyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-27-8 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 635325-28-9 CAPLUS
CN Benzoic acid, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 635325-29-0 CAPLUS
CN Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-(9CI) (CA INDEX NAME)

RN 635325-30-3 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-,
methyl ester (9CI) (CA INDEX NAME)

RN 635325-32-5 CAPLUS
CN Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-34-7 CAPLUS
CN Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-35-8 CAPLUS
CN Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 635325-36-9 CAPLUS
CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-(9CI) (CA INDEX NAME)

RN 635325-37-0 CAPLUS
CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-,
methyl ester (9CI) (CA INDEX NAME)

RN 635325-38-1 CAPLUS
CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

RN 635325-77-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-95-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2,4-difluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-76-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridiny1)-2-(4-fluoropheny1)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN 668481-77-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-1,6-dihydro-6-methyl-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-78-5 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(3-methylphenyl)-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-79-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(3-methylphenyl)-2-[3-methyl-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-80-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-1,6-dihydro-6-methyl-2-[3-methyl-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-81-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-1,6-dihydro-6-methyl-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-82-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(5-methyl-3-pyridinyl)-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-83-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-(5-methyl-3-pyridinyl)-2-[3-methyl-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-84-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-2-(4-iodophenyl)-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 668481-85-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

668481-86-5 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-1,6-dihydro-6-methyl-2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

668481-87-6 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl-4-(3-methylphenyl)- (9CI) (CA INDEX NAME) CN

RN

668481-88-7 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN

668481-89-8 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(6-ethoxy-3-pyridazinyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN 668481-90-1 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3,5-dimethylphenyl)-1,6-dihydro-6-methyl-4-(4-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 668481-91-2 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 668481-92-3 CAPLUS
CN Benzoic acid, 4-[4-(3-bromophenyl)-3,6-dihydro-6-methyl-3oxodipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-chloro-, methyl ester
(9CI) (CA INDEX NAME)

668481-93-4 CAPLUS
Benzoic acid, 4-[4-(3-bromophenyl)-3,6-dihydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-chloro- (9CI) (CA INDEX

668481-94-5 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-(4-nitrophenyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

668481-96-7 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-aminophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

668481-97-8 CAPLUS

2-Thiophenecarboxylic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

668481-98-9 CAPLUS CN

2-Thiophenecarboxylic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-4methyl- (9CI) (CA INDEX NAME)

668481-99-0 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME) CN

668482-00-6 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(methylsulfinyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN

668482-01-7 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-[3-(phenylmethoxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX CNNAME)

RN

668482-02-8 CAPLUS Benzoic acid, 4-[[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

MeO-C
$$CH_2 \qquad N \qquad N$$

$$N \qquad N$$

$$N \qquad N$$

$$N \qquad N$$

$$N \qquad N$$

668482-03-9 CAPLUS RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-CN6-(2-hydroxyethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

F<sub>3</sub>C 
$$\stackrel{\text{H}}{\longrightarrow}$$
  $\stackrel{\text{N}}{\longrightarrow}$   $\stackrel{\text{N}}{\longrightarrow}$   $\stackrel{\text{CH}_2-\text{CH}_2-\text{OH}}{\longrightarrow}$ 

668482-04-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(2-fluoro[1,1'-biphenyl]-4-yl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

668482-06-2 CAPLUS RNDipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,5-dihydro-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME) CN

668482-07-3 CAPLUS RNDipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-1,6-dihydro-6-methyl-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

MARPAT 140:163860

os GI

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ANSWER 2 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
1.4
    2004:100816 CAPLUS
ΑN
DN
    140:163860
    Preparation of dihydrodipyrazolopyridinylbenzamide and -sulfonamide
ΤI
     inhibitors of B7-1
    Green, Neal Jeffrey; Xiang, Jason Shaoyun; Davies, Audrey Molina; Chen,
IN
     Lihren
     Wyeth, John, and Brother Ltd., USA
PA
     U.S. Pat. Appl. Publ., 19 pp.
SO
     CODEN: USXXCO
     Patent
DT
                                                                       16734190
LΑ
    English
FAN.CNT 1
                                           APPLICATION NO. DATE
     PATENT NO.
                      KIND DATE
                                                           20030728
    US 2004024008
                       Al
                            20040205
                                           US 2003-629276
                            20020729
                      Ρ
PRAI US 2002-399146P
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The title compds. [I; X = CO, SO2; R1, R2 = H, alkyl, haloalkyl, AB cycloalkyl, etc.; R3 = H, F, Cl, Br, I; R4, R5 = H, NH2, (CH2)20(CH2)20(CH2)2NH2, etc.; or NR4R5 = (un)substituted 5-7 membered ring optionally containing one double bond, benzofused ring or an addnl. heteroatom selected from O, (un) substituted NH, S; R6 = (un) substituted Ph, cycloheteroalkyl, heteroaryl], useful for the immunotherapeutic treatment of transplant rejection or autoimmune disease, were prepared E.g., a multi-step synthesis of II which showed IC50 of 54 nM in test for B7-1/CD28 binding inhibition, was given. The pharmaceutical composition comprising the compound I is claimed.

T

II

635324-83-3P 635325-27-8P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of dihydrodipyrazolopyridinylbenzamide and -sulfonamide inhibitors of B7-1/CD28 binding)

635324-83-3 CAPLUS RNCN

Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

635325-27-8 CAPLUS RNBenzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

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635325-39-2P 635325-40-5P 635325-41-6P
           635325-42-7P 635325-43-8P 635325-44-9P
           635325-45-0P 635325-46-1P 635325-47-2P
           635325-48-3P 635325-49-4P 635325-50-7P
           635325-51-8P 635325-52-9P 635325-53-0P
           635325-54-1P 635325-55-2P 635325-57-4P
           635325-58-5P 635325-59-6P 635325-60-9P
           635325-61-0P 635325-62-1P 635325-63-2P
           635325-64-3P 635325-65-4P 635325-66-5P
           635325-67-6P 635325-68-7P 635325-69-8P
           654679-05-7P 654679-15-9P 654679-21-7P
           654679-27-3P 654679-32-0P 654679-41-1P
            654679-48-8P 654679-54-6P 654679-59-1P
            654679-71-7P 654679-76-2P 654679-91-1P
           654679-98-8P 654680-10-1P 654680-61-2P
            654680-66-7P 654680-75-8P 654680-80-5P
            654680-93-0P 654680-98-5P 654681-03-5P
            654681-08-0P 654681-13-7P 654681-17-1P
            654681-25-1P 654681-35-3P 654681-38-6P
            654681-43-3P 654681-45-5P 654681-46-6P
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            654682-14-1P 654682-17-4P 654682-20-9P
            654682-22-1P 654682-24-3P 654682-27-6P
            654682-28-7P 654682-30-1P 654682-32-3P
            654682-34-5P 654682-37-8P 654682-40-3P
            654682-42-5P 654682-44-7P 654682-46-9P
            654682-48-1P
            RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
            (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
                     (preparation of dihydrodipyrazolopyridinylbenzamide and -sulfonamide
                    inhibitors of B7-1/CD28 binding)
            635325-39-2 CAPLUS
RN
            Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-
CN
            \label{lem:continuous} (\texttt{trifluoromethyl}) \, \texttt{phenyl}] \, \texttt{dipyrazolo[3,4-b:3',4'-d]} \, \texttt{pyridin-2(1H)-yl]-N-(3-h)} \, \text{where } \, \texttt{dipyrazolo[3,4-b:3',4'-d]} \, \text{pyridin-2(1H)-yl]-N-(3-h)} \, \text{where } \, \texttt{dipyrazolo[3,4-b:3',4'-d]} \, \text{pyridin-2(1H)-yl]-N-(3-h)} \, \text{for all } \, \texttt{dipyrazolo[3,4-b:3'-d]} \, \text{for all
            hydroxypropyl) - (9CI) (CA INDEX NAME)
```

HO- 
$$(CH_2)_3$$
-NH-C H N N Me

(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-methoxypropyl)- (9CI) (CA INDEX NAME)

MeO - 
$$(CH_2)_3$$
 -  $NH$  -  $C$   $H$   $N$   $N$   $Me$ 

RN 635325-41-6 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-methoxypropyl)- (9CI) (CA INDEX NAME)

MeO- (CH<sub>2</sub>)<sub>3</sub>-NH-C 
$$\stackrel{\text{H}}{\underset{\text{N}}{|}}$$
  $\stackrel{\text{N}}{\underset{\text{N}}{|}}$   $\stackrel{\text{N}}{\underset{\text{N}}{|}}$   $\stackrel{\text{N}}{\underset{\text{N}}{|}}$ 

RN 635325-42-7 CAPLUS
CN Piperazine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]4-methyl- (9CI) (CA INDEX NAME)

RN 635325-43-8 CAPLUS
CN Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 635325-44-9 CAPLUS
CN Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluorobenzoyl]- (9CI) (CA INDEX NAME)

N C F N N Me

RN 635325-45-0 CAPLUS
CN Morpholine, 4-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

$$\bigcap_{0} \bigcap_{N} \bigcap_{N$$

RN 635325-46-1 CAPLUS CN Pyrrolidine, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 635325-47-2 CAPLUS
CN Pyrrolidine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 635325-48-3 CAPLUS
CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-49-4 CAPLUS
CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-50-7 CAPLUS
CN D-Proline, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-51-8 CAPLUS
CN L-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-52-9 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-53-0 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-54-1 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-55-2 CAPLUS
CN Isoquinoline, 2-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ N & - C & \\ & & \\ N & \\ & & \\ \end{array}$$

RN 635325-57-4 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(3,4-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

HO CH<sub>2</sub>-NH-C N N Me 
$$F_3C$$

635325-58-5 CAPLUS RN

Benzamide, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(3,4'-d]pyrid dihydroxyphenyl) methyl] - (9CI) (CA INDEX NAME)

635325-59-6 CAPLUS
Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(4-hydroxy-3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{OMe} \\ \mathsf{HO} \\ \mathsf{CH_2-NH-C} \\ \\ \mathsf{N} \\ \mathsf{N} \\ \mathsf{N} \\ \mathsf{N} \\ \mathsf{Me} \\ \\ \mathsf{N} \\ \mathsf{N}$$

RN

635325-60-9 CAPLUS Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(lH)-yl]-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)CN

635325-61-0 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-62-1 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-63-2 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-64-3 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(methoxymethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO-CH}_2 & \text{N} & \text{N} \\ \text{NH-C} & \text{N} & \text{N} \\ \text{N} & \text{N} & \text{Me} \\ \end{array}$$

RN

635325-65-4 CAPLUS Benzoic acid, 3-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

635325-66-5 CAPLUS RN

Benzamide, N-(3-acetylphenyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

635325-67-6 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

635325-68-7 CAPLUS RN

Benzamide, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-69-8 CAPLUS
CN Morpholine, 4-[5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluorobenzoyl]- (9CI) (CA INDEX NAME)

RN 654679-05-7 CAPLUS
CN Benzoic acid, 4-chloro-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

RN 654679-15-9 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN

654679-21-7 CAPLUS Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl) phenyl] dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2,2-dimethoxyethyl)-N-methyl- (9CI) (CA INDEX NAME)

RN

654679-27-3 CAPLUS Thiazolidine, 3-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

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654679-32-0 CAPLUS RN

Thiomorpholine, 4-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

654679-41-1 CAPLUS RN

Benzamide, N-(cyclopropylmethyl)-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN (CA INDEX NAME)

RN 654679-48-8 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxyethyl)-N-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{N} \\ \text{HO-CH}_2\text{-CH}_2\text{-N-C} & \text{N} \\ \text{O} & \text{N} \\ \end{array}$$

RN 654679-54-6 CAPLUS
CN 1H-Indole-3-carboxylic acid, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 654679-59-1 CAPLUS
CN Benzamide, N-[(4-aminophenyl)methyl]-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

RN 654679-71-7 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxypropyl)- (9CI) (CA INDEX NAME)

RN 654679-76-2 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{MeO-CH_2-CH_2-NH-C} \\ & \mathsf{N} \\ & \mathsf{N} \end{array}$$

RN 654679-91-1 CAPLUS
CN 2-Pyrrolidinemethanol, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

654679-98-8 CAPLUS Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

654680-10-1 CAPLUS RN

4-Piperidinecarboxylic acid, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-, methyl ester (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

654680-61-2 CAPLUS RN

3-Piperidinemethanol, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

654680-66-7 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(4-hydroxybutyl)- (9CI) (CA INDEX NAME) CN

RN 654680-75-8 CAPLUS
CN Benzamide, N-(5-aminopentyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

$$H_2N-(CH_2)_5-NH-C$$
 $H_2N-(CH_2)_5-NH-C$ 
 $H_1$ 
 $H_2$ 
 $H_2$ 
 $H_1$ 
 $H_2$ 
 $H_2$ 
 $H_3$ 
 $H_4$ 
 $H_4$ 

RN 654680-80-5 CAPLUS
CN Morpholine, 4-[2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 654680-93-0 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(5,6,7,8-tetrahydro-5-hydroxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

10629227

RN 654680-98-5 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, hydrazide (9CI) (CA INDEX NAME)

RN 654681-03-5 CAPLUS
CN Glycine, N-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], methyl ester (9CI) (CA INDEX NAME)

RN 654681-08-0 CAPLUS
CN Benzamide, N-[2-[2-(2-aminoethoxy)ethoxy]ethyl]-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

654681-13-7 CAPLUS RN

Benzamide, N-(3,4-difluorophenyl)-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

RN

654681-17-1 CAPLUS

Benzoic acid, 3-[[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & H & N \\ \hline \\ EtO-C & NH-C & N & N \\ \hline \\ O & NH-C & N \\ \end{array}$$

RN

654681-25-1 CAPLUS
Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

654681-35-3 CAPLUS RN4-Piperidinecarboxylic acid, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

654681-38-6 CAPLUS RN

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

HO- 
$$CH_2$$
-  $CH_2$ 

NH-  $C$ 

NH-  $C$ 

NH-  $C$ 

NH-  $C$ 

NH-  $C$ 

RN

654681-43-3 CAPLUS
Piperidine, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-3-methyl- (9CI) (CA INDEX NAME) CN

654681-45-5 CAPLUS

3-Piperidinecarboxamide, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-N,N-diethyl- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} C & O & O & H & N \\ Et_2N-C & N & C & N & N \\ \hline \\ N & N & N & Me \\ \hline \\ N & N & N & Me \\ \end{array}$$

RN 654681-46-6 CAPLUS

4-Piperidinol, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

654681-49-9 CAPLUS RN

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN $(\texttt{trifluoromethyl}) \, \texttt{phenyl}] \, \texttt{dipyrazolo} \, [\, 3\,,\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, \texttt{pyridin} \, -\, 2\,(\, 1\,H)\,\,-\, y\,l\,] \,\, -\, N\,-\, [\, (\, 4\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,] \,\, +\, 2\,(\, 2\,-\, b\,:\, 3\,'\,,\, 4\,'\,-\, d\,:\, 3\,'\,,\, 4\,'$ methoxyphenyl) methyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{O} & \text{H} & \text{N} \\ \text{CH}_2-\text{NH}-\text{C} & \text{N} & \text{N} \\ \text{O} & \text{N} & \text{N} \end{array}$$

654681-52-4 CAPLUS

RN

Benzamide, N-(2-cyanoethyl)-3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl) phenyl] dipyrazolo [3,4-b:3',4'-d] pyridin-2 (1H)-yl]-Nmethyl- (9CI) (CA INDEX NAME)

10629227

RN 654681-55-7 CAPLUS
CN Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 654681-60-4 CAPLUS CN D-Proline, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 654681-63-7 CAPLUS
CN Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 654681-68-2 CAPLUS

Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

654681-70-6 CAPLUS RN

Benzamide, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

654681-75-1 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

$$H_2N-C$$
 $H_2N-C$ 
 $H$ 

RN

CNhydroxyphenyl) - (9CI) (CA INDEX NAME)

10629227

654681-81-9 CAPLUS RN

Benzamide, N-(2-cyanoethyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-methyl- (9CI) (CA INDEX NAME)

654681-84-2 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME) CN

654681-86-4 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN

654681-88-6 CAPLUS
Benzamide, N-(cyclopropylmethyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

RN

654681-90-0 CAPLUS Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2hydroxypropyl) - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{O} \\ \text{Me-CH-CH}_2\text{-NH-C} & \text{H} & \text{N} \\ \\ \text{N} & \text{N} & \text{Me} \end{array}$$

654681-92-2 CAPLUS RN

Thiomorpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

654681-94-4 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 654681-96-6 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-3-pyridinyl- (9CI) (CA INDEX NAME)

RN 654681-98-8 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2,2-dimethoxyethyl)-N-methyl- (9CI) (CA INDEX NAME)

RN 654682-02-7 CAPLUS
CN Benzamide, N-(3,4-difluorophenyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI)
(CA INDEX NAME)

654682-04-9 CAPLUS RN

Thiazolidine, 3-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN

654682-06-1 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)-2-methylphenyl]- (9CI) (CA INDEX NAME)

654682-08-3 CAPLUS RN

Benzamide, N-(3-amino-3-oxopropyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-CNmethyl- (9CI) (CA INDEX NAME)

RN

654682-10-7 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[2-CN(hydroxymethyl)phenyl] - (9CI) (CA INDEX NAME)

654682-12-9 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

654682-14-1 CAPLUS RN

3-Piperidinecarboxamide, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-N,N-diethyl- (9CI) (CA INDEX NAME) CN

RN654682-17-4 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(dimethylamino)propyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_2\text{N-} \text{(CH}_2\text{)}_3 - \text{NH-C} \\ \\ \\ \text{N} \\ \\ \text{Me} \\ \\ \\ \text{N} \\ \\ \text{N$$

654682-20-9 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(4fluorophenyl) methyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN

654682-22-1 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-CNhydroxyethyl) - N-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & \text{HO-CH}_2\text{-CH}_2\text{-N-C} \\ & \text{N} \\ & \text{N} \\ & \text{Me} \\ & \text{N} \\ & \text{Me} \\ & \text{N} \\ & \text{Me} \\ & \text{N} \\ & \text{N} \\ & \text{N} \\ & \text{Me} \\ & \text{N} \\$$

654682-24-3 CAPLUS RN

4-Piperidinol, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl)dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

RN 654682-27-6 CAPLUS
CN 3-Piperidinol, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

HO N C 
$$\frac{1}{N}$$
  $\frac{1}{N}$   $\frac{1}{N}$   $\frac{1}{N}$   $\frac{1}{N}$   $\frac{1}{N}$   $\frac{1}{N}$   $\frac{1}{N}$   $\frac{1}{N}$ 

RN 654682-28-7 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(5-hydroxypentyl)- (9CI) (CA INDEX NAME)

HO- 
$$(CH_2)_5$$
-NH-C

N

N

N

Me

RN 654682-30-1 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3,4-dihydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 654682-32-3 CAPLUS

CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 654682-34-5 CAPLUS

CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxypropyl)phenyl]- (9CI) (CA INDEX NAME)

RN 654682-37-8 CAPLUS

CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(5-hydroxypentyl)- (9CI) (CA INDEX NAME)

RN 654682-40-3 CAPLUS

CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 654682-42-5 CAPLUS
CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

RN 654682-44-7 CAPLUS
CN Glycine, N-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]phenyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & O & O \\ \hline MeO-C-CH_2-NH-S & O & N & N \\ \hline O & N & N & N \\ \hline O & N & N & N \\ \hline \end{array}$$

RN 654682-46-9 CAPLUS
CN Benzenesulfonamide, N-(cyclopropylmethyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl](9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-NH-S & H & N \\ \hline \\ O & N & N \\ \hline \\ O & F_3C \\ \end{array}$$

RN 654682-48-1 CAPLUS

CN Glycine, N-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

IT 654682-52-7P 654682-55-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of dihydrodipyrazolopyridinylbenzamide and -sulfonamide inhibitors of B7-1/CD28 binding)

RN 654682-52-7 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridine-1(2H)-carboxylic acid,
2-[4-[[[(1,1-dimethylethoxy)carbonyl]amino]sulfonyl]phenyl]-3,6-dihydro-6methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

RN 654682-55-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridine-1(2H)-carboxylic acid, 3,6-dihydro-2-[4-[[(5-hydroxypentyl)amino]sulfonyl]phenyl]-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

## 10629227

ΑN 2003:427773 CAPLUS DN140:42073 ΤI Structure-activity studies of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones binding to the immune regulatory protein B7.1 AU Green, Neal J.; Xiang, Jason; Chen, Jing; Chen, Lihren; Davies, Audrey M.; Erbe, Dave; Tam, Steve; Tobin, James F. CS Department of Chemical Sciences, Wyeth Research, Cambridge, MA, 02140, USA SO Bioorganic & Medicinal Chemistry (2003), 11(13), 2991-3013 CODEN: BMECEP; ISSN: 0968-0896 PΒ Elsevier Science Ltd.  $\mathtt{DT}$ Journal LΑ English GI

I

AB The interaction of co-stimulatory mols. on T cells with B7 mols. on antigen presenting cells plays an important role in the activation of naive T cells. Consequently, agents that disrupt these interactions should have applications in treatment of transplant rejection as well as autoimmune diseases. To this end, specific small mol. inhibitors of human B7.1 were identified and characterized. Herein, we report the identification of potent small mol. inhibitors of the B7.1-CD28 interaction. In a high-throughput screen we identified several leads that prevented the interaction of B7.1 with CD28 with activities in the nanomolar to low micromolar range. One of these, the dihydrodipyrazolopyridinone I, was subsequently shown to bind the V-like domain of human B7.1 at equimolar stoichiometry. With this as a starting point, we report here the synthesis and initial in vitro structure-activity relationships of a series of these compds. 635324-71-9 635325-69-8 635325-95-0 RL: PAC (Pharmacological activity); BIOL (Biological study)

(preparation and structure-activity relationship of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones as inhibitors of the B7.1-CD28 interaction in T cells) 635324-71-9 CAPLUS

RN

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-phenyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

635325-69-8 CAPLUS

Morpholine, 4-[5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethy1)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2fluorobenzoyl] - (9CI) (CA INDEX NAME)

RN 635325-95-0 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2,4-difluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

IT 443146-92-7P 635324-87-7P 635324-90-2P

635324-95-7P 635325-20-1P 635325-21-2P

635325-27-8P 635325-28-9P 635325-29-0P

635325-32-5P 635325-35-8P 635325-36-9P

635325-38-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure-activity relationship of a series of dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones as inhibitors of the B7.1-CD28 interaction in T cells)

RN 443146-92-7 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{N} & \text{N} \\ \hline & \text{N} & \text{N} \\ \hline & \text{N} & \text{N} \\ \hline & \text{F}_3\text{C} & \\ \end{array}$$

RN 635324-87-7 CAPLUS

CN Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

635324-90-2 CAPLUS RN

Benzonitrile, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME) CN

RN

635324-95-7 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-CN 6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

635325-20-1 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

635325-21-2 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,5-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

RN

635325-27-8 CAPLUS
Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN(CA INDEX NAME)

RN

635325-28-9 CAPLUS
Benzoic acid, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

635325-29-0 CAPLUS
Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl) phenyl] dipyrazolo[3,4-b:3',4'-d] pyridin-2(1H)-yl]-2fluoro- (9CI) (CA INDEX NAME)

635325-32-5 CAPLUS
Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN

635325-35-8 CAPLUS Benzoic acid, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

$$HO_2C$$
 $HO_2C$ 
 $HO_2$ 

RN 635325-36-9 CAPLUS

CNBenzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro- (9CI) (CA INDEX NAME)

$$HO_2C$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

635325-38-1 CAPLUS
Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-4,4]] (trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2fluoro-, methyl ester (9CI) (CA INDEX NAME)

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443146-93-8P 635324-72-0P 635324-73-1P
     635324-74-2P 635324-75-3P 635324-76-4P
     635324-77-5P 635324-79-7P 635324-82-2P
     635324-83-3P 635324-84-4P 635324-85-5P
     635324-86-6P 635324-88-8P 635324-91-3P
     635324-92-4P 635324-93-5P 635324-94-6P
     635324-96-8P 635324-97-9P 635324-98-0P
     635324-99-1P 635325-03-0P 635325-05-2P
     635325-06-3P 635325-07-4P 635325-11-0P
     635325-13-2P 635325-19-8P 635325-23-4P
     635325-25-6P 635325-30-3P 635325-31-4P
     635325-34-7P 635325-37-0P 635325-39-2P
     635325-40-5P 635325-41-6P 635325-42-7P
     635325-43-8P 635325-44-9P 635325-45-0P
     635325-46-1P 635325-47-2P 635325-48-3P
     635325-49-4P 635325-50-7P 635325-51-8P
     635325-52-9P 635325-53-0P 635325-54-1P
     635325-55-2P 635325-56-3P 635325-57-4P
     635325-58-5P 635325-59-6P 635325-60-9P
     635325-61-0P 635325-62-1P 635325-63-2P
     635325-64-3P 635325-65-4P 635325-66-5P
     635325-67-6P 635325-68-7P 635325-77-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (preparation and structure-activity relationship of a series of
        dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones as inhibitors of the B7.1-CD28
        interaction in T cells)
RN
     443146-93-8 CAPLUS
CN
    Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-
     6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)
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RN 635324-72-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)
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RN 635324-73-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-74-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-chloro-4-fluorophenyl)1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-75-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(2-fluorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-76-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-[3(trifluoromethyl)phenyl]-2-[4-(trifluoromethyl)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 635324-77-5 CAPLUS
CN 2-Thiophenecarboxylic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-5-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CO}_2\text{H} & \text{H} & \text{N} \\ \text{N} & \text{N} & \text{N} \\ \text{Me} & \text{O} & \text{N} & \text{Me} \\ \end{array}$$

RN 635324-79-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(1,6-dihydro-6-oxo-3-pyridazinyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-82-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[4-(1,1-dimethylethyl)phenyl]-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

RN 635324-83-3 CAPLUS
CN Benzenesulfonamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) (CA INDEX NAME)

RN 635324-84-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-[4-(phenylmethoxy)phenyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635324-85-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-[1,1'-biphenyl]-4-yl-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RNCN

635324-86-6 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-2-[4-(hydroxymethyl)phenyl]-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN

635324-88-8 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN635324-91-3 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-bromophenyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

RN

635324-92-4 CAPLUS
Benzoic acid, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME) CN

635324-93-5 CAPLUS

Benzamide, 3-[2-(3-fluorophenyl)-1,2,3,6-tetrahydro-6-methyl-3-oxodipyrazolo[3,4-b:3',4'-d]pyridin-4-yl]- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN

635324-94-6 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(5-bromo-3-pyridinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

RN

635324-96-8 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3-aminophenyl)-2-(4-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

635324-97-9 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-phenyl- (9CI) (CA INDEX NAME) CN

RN 635324-98-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-4-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

RN

635324-99-1 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-pyridinyl)- (9CI) (CA INDEX NAME) CN

RN 635325-03-0 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(3,5-dichlorophenyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME)

635325-05-2 CAPLUS

RN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-thienyl)- (9CI) (CA INDEX NAME) CN

## 10629227

RN635325-06-3 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-4-(3-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

635325-07-4 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(1,3-benzodioxol-5-yl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

RN

635325-11-0 CAPLUS
Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 4-(2,6-dimethyl-4-morpholinyl)-2-(3-fluorophenyl)-1,6-dihydro-6-methyl- (9CI) (CA INDEX NAME) CN

RN635325-13-2 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-1,6-dimethyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME) CN

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-phenyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-23-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-2-(4-fluorophenyl)-1,6-dihydro-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-25-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,6-dihydro-6-propyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-30-3 CAPLUS
CN Benzoic acid, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & H & N \\ \hline MeO-C & N & N \\ \hline O & N & N \\ \hline \end{array}$$

RN635325-31-4 CAPLUS

Benzoic acid, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN

635325-34-7 CAPLUS Benzoic acid, 5-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

635325-37-0 CAPLUS Benzoic acid, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-, methyl ester (9CI) (CA INDEX NAME)

MeO-C 
$$\stackrel{\text{N}}{=}$$
  $\stackrel{\text{N}}{=}$   $\stackrel{\text{N}}{=}$ 

635325-39-2 CAPLUS RN

CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl) phenyl] dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)

HO- 
$$(CH_2)_3$$
-NH-C

RN 635325-40-5 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-methoxypropyl)- (9CI) (CA INDEX NAME) CN

MeO- (CH<sub>2</sub>)<sub>3</sub>-NH-C 
$$\stackrel{\text{H}}{\underset{\text{N}}{\parallel}}$$
  $\stackrel{\text{N}}{\underset{\text{N}}{\parallel}}$   $\stackrel{\text{N}}{\underset{\text{N}}{\parallel}}$   $\stackrel{\text{N}}{\underset{\text{N}}{\parallel}}$ 

RN635325-41-6 CAPLUS

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(3-CNmethoxypropyl) - (9CI) (CA INDEX NAME)

MeO- (CH<sub>2</sub>)<sub>3</sub>-NH-C 
$$\stackrel{\text{H}}{\underset{\text{N}}{\parallel}}$$
  $\stackrel{\text{H}}{\underset{\text{N}}{\parallel}}$   $\stackrel{\text{N}}{\underset{\text{N}}{\parallel}}$   $\stackrel{\text{Me}}{\underset{\text{N}}{\parallel}}$ 

RN

635325-42-7 CAPLUS
Piperazine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-4-methyl- (9CI) (CA INDEX NAME) CN

635325-43-8 CAPLUS Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

635325-44-9 CAPLUS Morpholine, 4-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluorobenzoyl]- (9CI) (CA INDEX NAME)

RN

635325-45-0 CAPLUS Morpholine, 4-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN

635325-46-1 CAPLUS
Pyrrolidine, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 635325-47-2 CAPLUS
CN Pyrrolidine, 1-[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

RN 635325-48-3 CAPLUS
CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl], methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-49-4 CAPLUS CN D-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-50-7 CAPLUS
CN D-Proline, 1-[2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-51-8 CAPLUS CN L-Proline, 1-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 635325-52-9 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-53-0 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph} & \text{CH}_2 - \text{NH} - \text{C} \\ \hline \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{Me} \\ \end{array}$$

RN 635325-54-1 CAPLUS
CN Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 635325-55-2 CAPLUS
CN Isoquinoline, 2-[3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

RN 635325-56-3 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-0xo-4-[3-methyl-3-[3-methyl(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(3,4-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

RN 635325-57-4 CAPLUS

CN

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3- $(trifluoromethyl)\,phenyl]\,dipyrazolo\,[3,4-b:3',4'-d]\,pyridin-2\,(1H)\,-yl]\,-N-\,[\,(3,4-b:3',4'-d)\,pyridin-2\,(2H)\,-y$ dihydroxyphenyl)methyl] - (9CI) (CA INDEX NAME)

RN 635325-58-5 CAPLUS

Benzamide, 2-chloro-5-[3,6-dihydro-6-methyl-3-oxo-4-[3- $(\texttt{trifluoromethyl}) \, \texttt{phenyl}] \, \texttt{dipyrazolo} \, [3,4-b:3',4'-d] \, \texttt{pyridin-2(1H)-yl}] \, -N-[(3,4-b:3',4'-d)] \, +N-[(3,4-b:3',4'-d)] \, +N-[(3,4-b:3',4'-d)$ dihydroxyphenyl)methyl] - (9CI) (CA INDEX NAME)

RN

CN(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[(4hydroxy-3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \text{HO} \\ \text{CH}_2 - \text{NH} - \text{C} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{Me} \\ \\ \text{N} \\ \\ \text{N$$

RN

635325-60-9 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c} \text{HO-CH}_2\text{-CH}_2\\ \text{NH-C} \end{array}$$

RN

635325-61-0 CAPLUS
Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-2-fluoro-N-[4-(2-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME) CN

635325-62-1 CAPLUS RN

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN635325-63-2 CAPLUS

Benzamide, 3-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(hydroxymethyl)phenyl]- (9CI) (CA INDEX NAME)

RN635325-64-3 CAPLUS

Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-CN  $(\texttt{trifluoromethyl}) \, \texttt{phenyl}] \, \texttt{dipyrazolo} \, [\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2} \, (\texttt{1H}) \, -\texttt{y1}] \, -\texttt{N-} \, [\texttt{3-dipyrazolo}] \, [\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2} \, (\texttt{1H}) \, -\texttt{y1}] \, -\texttt{N-} \, [\texttt{3-dipyrazolo}] \, [\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2} \, (\texttt{1H}) \, -\texttt{y1}] \, -\texttt{N-} \, [\texttt{3-dipyrazolo}] \, [\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2} \, (\texttt{1H}) \, -\texttt{y1}] \, -\texttt{N-} \, [\texttt{3-dipyrazolo}] \, [\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2} \, (\texttt{1H}) \, -\texttt{y1}] \, -\texttt{N-} \, [\texttt{3-dipyrazolo}] \, [\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2} \, (\texttt{3,4-b:3',4'-d}] \, \texttt{pyridin-2} \, (\texttt{3,4-b:3',4'-d}) \, \texttt{pyridin-2} \, (\texttt{3,4-b:3',4'-d})$ (methoxymethyl)phenyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO-CH}_2 & \text{O} & \text{N} & \text{N} \\ \hline & \text{N} & \text{N} & \text{Me} \\ \hline & \text{N} & \text{N} & \text{Me} \\ \end{array}$$

RN

635325-65-4 CAPLUS Benzoic acid, 3-[[4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

MeO-C 
$$NH-C$$
  $NH-C$   $N$ 

635325-66-5 CAPLUS
Benzamide, N-(3-acetylphenyl)-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]- (9CI) CN (CA INDEX NAME)

RN 635325-67-6 CAPLUS
CN Benzamide, 4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-68-7 CAPLUS
CN Benzamide, 2-chloro-4-[3,6-dihydro-6-methyl-3-oxo-4-[3-(trifluoromethyl)phenyl]dipyrazolo[3,4-b:3',4'-d]pyridin-2(1H)-yl]-N-[3-(1-hydroxyethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-77-8 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-2-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-09-6 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridine-3,4-dione, 2-(3-fluorophenyl)-1,2,5,6-tetrahydro-6-methyl- (9CI) (CA INDEX NAME)

RN 635325-22-3 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-fluorophenyl)-1,5-dihydro1-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 635325-24-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-2-(4-fluorophenyl)-1,6-dihydro-1-(phenylmethyl)-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

# RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:209621 CAPLUS

DN 137:103581

TI Small molecule ligands define a binding site on the immune regulatory protein B7.1

AU Erbe, David V.; Wang, Suyue; Xing, Yuzhe; Tobin, James F.

CS Wyeth Research, Cambridge, MA, 02140, USA

SO Journal of Biological Chemistry (2002), 277(9), 7363-7368 CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DT Journal

LA English

AB The interaction of co-stimulatory mols. on T cells with B7 mols. on antigen presenting cells plays an important role in the activation of naive T cells. Consequently, agents that disrupt these interactions should have applications in treatment of transplant rejection as well as autoimmune diseases. To this end, specific small mol. inhibitors of human B7.1 were identified and characterized. These compds. inhibit the binding of B7.1 to both CD28 and CTLA4. Both classes of compds. appear to bind the same site, a relatively small portion of the GFCC'C'' face of the N-terminal V-set domain of human B7.1, not present in the homologous B7.2 or even mouse B7.1. This site may represent a rare hot spot for small mol. antagonist design of inhibitors of cell-cell interactions, whose ligands may yield leads for the development of novel immunomodulatory medicines.

IT 443146-92-7 443146-93-8

RL: PAC (Pharmacological activity); BIOL (Biological study) (small mol. ligands define a binding site on the immune regulatory protein B7.1)

RN 443146-92-7 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(4-chlorophenyl)-1,6-dihydro-6-methyl-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 443146-93-8 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 2-(3-fluorophenyl)-1,6-dihydro-6-methyl-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

#### RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

T.4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:131636 CAPLUS

128:192869 DN

Synthesis of  $\beta\text{-D-ribonucleosides}$  derived from dipyrazolo[3,4-b:3'4'-ΤI d]pyridin-3-one system

Bernardino, Alice M. R.; Nogueira, Christiane M.; de O. Lepesch, Carla M.; Gomes, Claudia R. B.; Schmitz, Francis J.; Romeiro, Gilberto A.; de S. Pereira, Helena; de P. P. Frughlhetti, Isabel C.; de Oliveira, Mara R. P.; de Souza, maria C. B. V.; Lee, Marietta Y. W. T.; Chaves, Salma A.; Ferreira, Vitor F.

Departamento de Quimica Organica, Instituto de Quimica, Universidade CS

Federal Fluminense, Niteroi, 24020-150, Brazil Heterocyclic Communications (1997), 3(6), 527-534 SO CODEN: HCOMEX; ISSN: 0793-0283

PB Freund Publishing House Ltd.

DTJournal

LΑ English

The new ribonucleosides 8-methyl-2,6-diphenyl-5-(2,3,5-tri-0-benzoyl-AB  $\beta$ -D-ribofuranosyl)-2H,6H-dipyrazolo[3,4-b:3<sup>1</sup>4'-d]pyridin-3(5H)-one and 8-methyl-2-(p-nitrophenyl)-6-phenyl-5-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-2H,6H-dipyrazolo[3,4-b:3'4'-d]pyridin-3(5H)-one were prepared from stannic chloride-catalyzed ribosylations of the corresponding heterocycles. Attempts of de-O-benzovlation failed to give the free ribosides. The effect of these compds. on the catalytic activities of reverse transcriptase from recombinant immunodeficiency virus type 1 was evaluated. Some compds. inhibited the RNA dependent DNA polymerase activity of the enzyme by more than 50% at a concentration of 70  $\mu M. \,$ contrast, human placental DNA polymerase activities  $\alpha$  and  $\epsilon$ were unaffected by this concentration The structures of the nucleosides are supported by 1D and 2D-NMR techniques (nodes, HMBC and HMQC expts.). 81153-40-4P 203719-80-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation of ribonucleosides derived from a dipyrazolopyridinone system)

81153-40-4 CAPLUS

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-2,6diphenyl- (9CI) (CA INDEX NAME)

RN 203719-80-6 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-2-(4nitrophenyl) -6-phenyl- (9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN ΑN 1982:142751 CAPLUS 96:142751 Tricyclic heteroatomic ring systems. III. Synthesis of 1H,6H-dipyrazolo[3,4-b:3',4'-d]pyridin-3-ones TΙ Khan, Misbahul A.; Pedrotti, Francisco Secao Quim., Inst. Mil. Eng., Rio de Janeiro, 22290, Brazil Monatshefte fuer Chemie (1982), 113(1), 123-7 ΑU CS SO CODEN: MOCMB7; ISSN: 0026-9247 DΤ Journal LΑ English OS CASREACT 96:142751 GT

RN 81153-32-4 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-methyl-8-phenyl(9CI) (CA INDEX NAME)

RN 81153-33-5 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6,8-diphenyl-(9CI) (CA INDEX NAME)

RN 81153-34-6 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-6-phenyl-(9CI) (CA INDEX NAME)

RN 81153-35-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1,6,8-trimethyl(9CI) (CA INDEX NAME)

RN 81153-36-8 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1,6-dimethyl-8-phenyl- (9CI) (CA INDEX NAME)

RN 81153-37-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6,8-diphenyl- (9CI) (CA INDEX NAME)

RN 81153-38-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1,8-dimethyl-6-phenyl- (9CI) (CA INDEX NAME)

RN 81153-39-1 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6-phenyl-(9CI) (CA INDEX NAME)

RN 81153-41-5 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-8-methyl-1,6-diphenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1978:517633 CAPLUS

DN 89:117633

TI Hydrolysis and subsequent cyclization of etazolate hydrochloride and related compounds in aqueous solutions: application of PMR and mass spectrometry in accelerated stability studies

AU Puar, Mohindar S.; Funke, Phillip T.; Cohen, Allen I.

CS Squibb Inst. Med. Res., Princeton, NJ, USA

SO Journal of Pharmaceutical Sciences (1978), 67(6), 850-3 CODEN: JPMSAE; ISSN: 0022-3549

DT Journal

LA English

GI

The hydrolysis of etazolate-HCl (I) [35838-58-5], an inhibitor of cyclic AB nucleotide 3',5'-monophosphate phosphodiesterase that degrades cyclic adenosine 3',5'-monophosphate (cyclic AMP) to AMP, and related compds. was studied by PMR and mass spectrometry. The compds. underwent reversible acid-catalyzed hydrolysis in aqueous solns. at 60°, followed by cyclization to a major and a minor product formed by independent pathways. Under the exptl. conditions, the minor product was stable. The formation rate of the major product 6-ethyl-1,6-dihydrodipyrazolo[3,4-b:3',4'd]pyridin-3(2H)ione (II) [37649-55-1], was considerably greater than that of the minor component, 3-ethoxy-6-ethyl-1,6dihydrodipyrazolo[3,4-b:3',4'-d]pyridine (III) [51700-83-5]. For the 6-Me analog (IV) [67324-49-6] of etazolate, the rate of Me deuteration was considerably slower than the rate of cyclization. IΤ 37649-55-1

RL: BIOL (Biological study)

(etazolate hydrolysis-cyclization product)

RN 37649-55-1 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro- (9CI) (CA INDEX NAME)

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ANSWER 8 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1974:108514 CAPLUS
DN
     80:108514
     Dipyrazolo[3,4-b:3'4'-d]pyridine derivatives and their salts
ΤI
ΙN
     Hoehn, Hans; Denzel, Theodor
PA
     Chemische Fabrik von Heyden G.m.b.H.
     Ger. Offen., 37 pp.
SO
     CODEN: GWXXBX
DT
     Patent
LΑ
     German
FAN.CNT 1
     PATENT NO.
                       KIND DATE
                                             APPLICATION NO. DATE
                       ----
                                             -----
     DE 2333603
                       A1
                             19740131
                                             DE 1973-2333603 19730702
     US 3787430
                       Α
                             19740122
                                             US 1972-271477
                                                              19720713
     FR 2192831
                       A1
                             19740215
                                            FR 1973-25831
                                                               19730713
     JP 49051300
                       A2
                             19740518
                                             JP 1973-79725
                                                              19730713
PRAI US 1972-271477
                             19720713
     For diagram(s), see printed CA Issue.
    Tranquilizing and antiasthmatic dipyrazolopyridines I (R = H, Me, Et,
    CH2Ph, CH2CH2CHMe2, (CH2)3NMe2, COC6H4Cl-p; R1 = Ph, Me, NH2, OEt, OMe, OH, OCH2CH2CHMe2; R2 = Et, CH2Ph) were prepared Thus, 5-amino-1-
    ethylpyrazole was cyclized with EtOCH:C(COPh)CO2Et to give
    5-benzoyl-1-ethyl-4-hydroxy-1H-pyrazolo[3,4-b]pyridine, which was
    chlorinated and cyclized with N2H4 to I (R = H, R1 = Ph, R2 = Et).
    Treatment with C1(CH2)3NMe2 gave I (R = (CH2)3NMe2, R1 = Ph, R2 = Et).
    37649-62-0P 51700-79-9P 51700-81-3P
    51700-84-6P 51700-85-7P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and alkylation of)
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37649-62-0 CAPLUS

RN

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RN 51700-79-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-,
monopotassium salt (9CI) (CA INDEX NAME)
```

● F

RN 51700-81-3 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1-(2-furanylmethyl)-1,6-dihydro- (9CI) (CA INDEX NAME)

RN 51700-84-6 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-4,8-dimethyl- (9CI) (CA INDEX NAME)

RN 51700-85-7 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-4,8-dimethyl-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{N} \\ \hline \\ \text{HN} & \text{N} \\ \hline \\ \text{O} & \text{N} \end{array}$$

RN 51700-88-0 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-(3methylbutyl) - (9CI) (CA INDEX NAME)

RN 51700-90-4 CAPLUS Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-CN (phenylmethyl) - (9CI) (CA INDEX NAME)

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L4
    ANSWER 9 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN
    1972:514401 CAPLUS
DN
    77:114401
```

1,6-Dihydrodipyrazolo[3,4-b:3',4'-d]pyridine-3(2H)-ones TΙ

IN Hoehn, Hans; Schulze, Ernst

PAChemische Fabrik von Heyden G.m.b.H.

SO Ger. Offen., 21 pp.

CODEN: GWXXBX

DT Patent LΑ German

FAN.CNT 2

PATENT NO. KIND DATE APPLICATION NO. DATE ---------DE 2159600 Α 19720608 DE 1971-2159600 19711201 US 3669950 Α 19720613 US 1970-94179 19701201 PRAI US 1970-94179 19701201

GΙ

For diagram(s), see printed CA Issue. Seven title compds. (I, R = H, Me, CH2CH2OH, R1 = H, Ph, R2 = Et, CH2Ph) and their HCl salts, sedatives, tranquilizers, anxiolytics, and agents for increasing the cellular concentration of adenosine cyclic 3'5'-phosphate, were prepared Reaction of the 5-aminopyrazoles (II) with EtOCH:C(CO2Et)2 gave the di-Et [(5-pyrazolyl)-aminomethylene]malonates (III), which were cyclized in Ph2O at ≤250° to give the Et 4-hydroxy-1H-pyrazolo[3,4-b]pyridine-5-carboxylates (IV). These reacted either with EtI-K2CO3 to give IV 4-ethoxy analogs or with POCl3 to give IV 4-chloro analogs, either of which reacted with RNHNH2 or H2NNHR1 in EtOH in the presence of ZnCl2 to give the 4-hydrazino analogs, which were cyclized with Na in EtOH at reflux to give I. I (R = R1 = H) were methylated to give I (R = Me, R1 = H).

37649-55-1P 37649-58-4P 37649-61-9P 37649-62-0P 37649-63-1P 37649-64-2P IT 39022-83-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 37649-55-1 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro- (9CI)
(CA INDEX NAME)

RN 37649-58-4 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

## ●x HCl

RN 37649-61-9 CAPLUS

CN

Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-2-phenyl-(9CI) (CA INDEX NAME)

RN 37649-62-0 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-methyl(9CI) (CA INDEX NAME)

RN 37649-63-1 CAPLUS

CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 37649-64-2 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

## ●x HCl

```
ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
      1972:488501 CAPLUS
AN
DN
      77:88501
      Dipyrazolo[3,4-B:3',4'-D]-pyridin-3-ones
TI
 IN
      Hoehn, Hans; Schulze, Ernest
PΑ
      E. R. Squibb and Sons, Inc. U.S., 5 pp.
SO
      CODEN: USXXAM
DT
      Patent
LΑ
      English
FAN.CNT 2
      PATENT NO.
                        KIND DATE
                                               APPLICATION NO. DATE
      US 3669950
                         Α
                               19720613
                                               US 1970-94179
                                                                  19701201
      CA 947766
                         A1
                               19740521
                                               CA 1971-128355
                                                                  19711123
      GB 1374310
                               19741120
                                               GB 1971-55068
                                                                  19711126
      HU 164974
                         P
                               19740528
                                               HU 1971-SU693
                                                                  19711130
     DE 2159600
                         Α
                               19720608
                                               DE 1971-2159600
                                                                  19711201
      FR 2116469
                         Α5
                              19720713
                                               FR 1971-43127
                                                                  19711201
      FR 2116469
                         вı
                               19750418
      CH 540274
                         Α
                               19730928
                                               CH 1971-17467
                                                                  19711201
PRAI US 1970-94179
                               19701201
     For diagram(s), see printed CA Issue.
     Dipyrazolopyridinones (I, R = Et, PhCH2; R1 = H, Me, HOCH2CH2; R2 = H, Ph)
     useful as tranquilizers and for increasing intracellular concentration of cyclic
     AMP were prepared by cyclizing hydrazinopyrazolopyridinecarboxylates (II, R3
     = NHNH2, NHNHPh, NMeNH2, N(CH2CH2OH)NH2). Thus, 1-ethyl-5-aminopyrazole
     was condensed with EtOCH:C(CO2Et)2 to 84% Et 1-ethyl-5-
     pyrazolylaminomethylenemalonate which was cyclized to 92% II (R = Et, R3 =
     OH). O-Ethylation of II (R = Et, R3 = OH) and treatment with NH2NH2.H2O gave II (R = Et, R3 = NHNH2), which (10 g) was cyclized to I (R = Et, R1 =
     R2 = H); yield 8.5 g dihydrochloride.
     37649-55-1P 37649-58-4P 37649-61-9P 37649-62-0P 37649-63-1P 37649-64-2P
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
ВN
     37649-55-1 CAPLUS
     Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro- (9CI)
CN
     (CA INDEX NAME)
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RN 37649-58-4 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-6-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 37649-61-9 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-2-phenyl(9CI) (CA INDEX NAME)

RN 37649-62-0 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-methyl-(9CI) (CA INDEX NAME)

RN 37649-63-1 CAPLUS
CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 1,6-dihydro-1-methyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 37649-64-2 CAPLUS CN Dipyrazolo[3,4-b:3',4'-d]pyridin-3(2H)-one, 6-ethyl-1,6-dihydro-1-(2-

hydroxyethyl) ~ (9CI) (CA INDEX NAME)